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Researchers at the Southern Science Center (SSC) develop computer programs for the chemical laboratory. For instance, spectrophotometric absorbance determination of unknown compounds can be calculated and fitted to Beer's Law by using a least-squares fitting routine programmed in the form of a source program. The source program was developed with a modern approach to data analysis in beginner's all-purpose symbolic instruction code (BASIC) as a compiler language and can be imported into any standard version of the compiler language for execution.

The relation between absorbance and concentration, known as Beer's Law, is determined through the functional relation between the quantity measured in an absorption method (A) and the quantity sought (the analyte concentration, c). The Beer's relation can be expressed as

$$\log T = Ebc$$

where T is the transmittance (transmitted light or incident light), E is the molar extinction coefficient or absorptivity (liter/mole centimeters), b is the path length of the radiation through the absorbing medium (centimeters), and c is the concentration of the absorbing medium (moles/liter). When the concentration is expressed in moles per liter and b is in centimeters, the proportionality constant is called the molar absorptivity and is expressed as E.

Thus

$$A = Ebc = -\log T$$

where E has the units of $L \text{ cm}^{-1} \text{ mol}^{-1}$ and the percentage transmittance (%T) is

$$2 - \log \%T = -\log T = Ebc$$

$$A = 2 - \log \%T$$

The source program for the spectrophotometric calculation requires the concentrations and percentage transmissions of a given component in a series of standard solutions. Absorbances are calculated and fitted to Beer's Law with a least-squares fitting routine, and the concentrations of the unknowns for which the percentage transmissions have been measured are calculated.

The subroutine (contact the author to obtain) uses three subscripted variables: X(I) and Y(I) contain the absorbance and concentration, respectively, of the Ith known standard solution, whereas W(I) contains the statistical weight of that point, in this case unity. The linear least-squares subroutine is introduced; it calculates the least-squares slope and intercept and their uncertainties from a set of points X(I), Y(I), with weights W(I). This is based on one of the most widespread computer uses in chemistry that fits theoretical curves to experimental data. The simplest curve is a straight line, $y = a_0 + a_1x$ where a_0 is the intercept and a_1 is the slope. A straight line may be fitted to a set of data points (x_i, y_i) , $i = 1, 2, \dots, n$, with associated weighting factors, w_i , and the least-squares criterion as a measure of the goodness of the fit.

The source program described is useful for chemists and other related professionals because it provides a simple

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means of analyzing spectrophotometric absorbances and concentrations for unknown substances with a microcomputer. This source program may simplify, provide a new, or add an alternative means for calculating spectrophotometric data. The combination of Beer's Law and a least-squares fitting routine offers the ability to construct chemical and statistical probabilities of electronic spectra measuring the intensity of spectrophotometric absorption values. If the source program is used with MS-DOS QBasic, no additional cost is involved to develop this procedure. MS-DOS QBasic is the programming environment included with the disk operating system of IBM and compatible personal computers.

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